

NON-ANTI-HERMITIAN QUATERNIONIC QUANTUM MECHANICS

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The breakdown of Ehrenfest's theorem imposes serious limitations on quaternionic quantum mechanics (QQM). In order to determine the conditions in which the theorem is valid, we examined the conservation of the probability density, the expectation value and the classical limit for a non-anti-hermitian formulation of QQM. The results also indicated that the non-anti-hermitian quaternionic theory is related to non-hermitian quantum mechanics, and thus the physical problems described with both of the theories should be related.

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I. INTRODUCTION

Currently, quaternionic quantum mechanics (QQM) is a theory of anti-hermitian operators [1], and thus the mathematical framework of QQM has been developed using hermitian formalism of complex quantum mechanics (CQM) as a reference frame. However, several CQM structures have no exact equivalent in QQM. Consequently, the physical interpretation of the theories may differ dramatically.

In this study, we are interested in the specific discrepancy between the classical limits of hermitian CQM and anti-hermitian QQM. The Ehrenfest theorem states that the expectation values of position and linear momentum calculated through CQM obey a classical dynamics. The theorem thus postulates that quantum mechanics and classical mechanics are somewhat related, so that quantum dynamics must have a classical limit. Furthermore, it sets forth the background for proposing that quantum phenomena may be generated by fluctuations of classical quantities. Accordingly, the Ehrenfest theorem is a basic concept that enables the formulation of semi-classical quantum mechanics, with far-reaching consequences that are both conceptual and practical in nature. Consequently, the breakdown of the Ehrenfest theorem for anti-hermitian QQM [1] proves that the physical contents of hermitian CQM and anti-hermitian QQM are different, and thus the phenomena described by both theories are probably different.

We may conclude that QQM is either disconnected from classical mechanics, and thus QQM has no classical limit, or that within the classical limit of QQM there is a generalized, and unknown, classical theory. In this study, we propose another point of view, in which QQM is not an anti-hermitian generalization of hermitian CQM. In fact, we propose a non-anti-hermitian QQM as a generalization for non-hermitian CQM. Using this simple assumption, we were able to ascertain that the breakdown of Ehrenfest for non-anti-hermitian Hamilton operators is similar to the breakdown of the Ehrenfest theorem observed in non-hermitian CQM, and thus we expect that a link between non-hermitian CQM and non-anti-hermitian QQM may be established physically as well as mathematically. Furthermore, we shall see that the Ehrenfest theorem may be verified in the particular case where hermitian operators

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are considered for QQM. We hope that our results can increase the interest in QQM and enable us to understand which kind of physical phenomena may be described with it, if any.

This article is organized according to the two possible quaternionic wave equations that we consider, namely the left complex wave equation (LCWE) and the right complex wave equation (RCWE). In Section II we define the LCWE and study its fundamental properties, namely the continuity equation for the probability density, the expectation values and the Ehrenfest theorem. Furthermore, we study basic properties of hermitian Hamiltonians in QQM. In section III we repeat the results for RCWE and, in Section IV, we present our conclusions and future directions for research.

II. THE LEFT-COMPLEX WAVE EQUATION

Let us consider the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \mathcal{H}\Psi. \quad (1)$$

The left hand side of (1) admits two positions of the complex unit i , and hence we call (1) the left-complex wave equation (LCWE). In accordance with a previous study of the Aharonov-Bohm effect in QQM [2], we propose the quaternionic Hamiltonian operator

$$\mathcal{H} = -\frac{\hbar^2}{2m} (\nabla - Q)^2 + V. \quad (2)$$

Q is a pure imaginary quaternionic vector, and V is a quaternionic scalar potential. Using the symplectic notation we write

$$Q = \alpha i + \beta j \quad \text{and} \quad V = V_0 + V_1 j, \quad (3)$$

where α , β , V_0 and V_1 are complex. The anti-commuting quaternionic complex units i , j and k satisfy

$$ij = -ji = k \quad \text{and} \quad ijk = -1, \quad (4)$$

and further details about quaternions and their applications in physics may be found at [3]. The quaternionic Hamiltonian (2) is general and neither Hermiticity nor anti-Hermiticity are supposed. From the wave equation (1), we obtain the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot j = g, \quad (5)$$

where ρ is the probability density, j is the probability current density and g is the source of probability density. The terms of the continuity equation (5) are

$$\rho = \Psi\Psi^* \quad g = \frac{1}{\hbar} (iV^* - Vi)\rho, \quad j = \frac{1}{2m} \left[(\Pi\Psi)\Psi^* + ((\Pi\Psi)\Psi^*)^* \right] \quad \text{and} \quad \Pi\Psi = -i\hbar(\nabla - Q)\Psi, \quad (6)$$

where Π is the gauge-invariant quaternionic momentum operator. If the source term g is zero, there is neither source nor sink of probability, and this is an important consistency test. The source term g of (6) is zero when V_0 is real even for quaternionic potentials, and the exact correspondence between QQM and CQM in this case has led to the formulation of anti-Hermitian QQM. However, the conservation of the probability density does not preclude the existence of other sources of discrepancy between QQM and CQM, as we shall see for the Ehrenfest theorem. On the other hand, non-zero sources appear in non-Hermitian CQM [4, 5], particularly when complex scalar potentials are admitted, and then we shall research quaternionic potentials taking the non-hermitian complex case as our frame of reference.

Real V_0 potentials have been explored in non-anti-hermitian QQM with relative success [6–17]. However, we point out that (2) is neither hermitian nor anti-hermitian even for $V = 0$. This is an example that leads to the question of whether anti-hermiticity is really necessary for QQM. In order to obtain a quaternionic quantum theory with a well-defined classical limit, we take inspiration from complex quantum mechanics. The expectation value of the canonical momentum is defined by

$$\langle \Pi \rangle = m \int dx^3 j. \quad (7)$$

Using the quaternionic probability current from (6), we propose the expectation value for an arbitrary quaternionic operator \mathcal{O} to be

$$\langle \mathcal{O} \rangle = \frac{1}{2} \int dx^3 \left[(\mathcal{O}\Psi)\Psi^* + \left((\mathcal{O}\Psi)\Psi^* \right)^* \right]. \quad (8)$$

This definition generalizes the expectation value of CQM for two reasons. Firstly, because the usual definition is recovered when \mathcal{O} is hermitian and, secondly because (8) is real for every \mathcal{O} , regardless of its hermiticity. Let us then ascertain whether QQM is well-defined within the classical limit when the expectation value (8) is supposed. The time-derivative of the position operator \mathbf{r} gives

$$\frac{d\langle \mathbf{r} \rangle}{dt} = \frac{\langle \mathbf{\Pi} \rangle}{m} + \frac{2}{\hbar} \langle iV\mathbf{r} \rangle. \quad (9)$$

The second term of the right hand side of (9) shows that the position expectation value does not follow a classical evolution. However, this result is in agreement with non-hermitian CQM, where such a term is present, and thus we hypothesize that non-anti-hermitian QQM may generalize non-hermitian CQM. By way of clarification, we notice that

$$2\langle iV\mathbf{r} \rangle = \langle (V^*i - iV)\mathbf{r} \rangle \quad (10)$$

is identical to zero for real V_0 , considering V as defined in (3). This means that $\langle \mathbf{r} \rangle$ obeys classical dynamics, and consequently satisfies the Ehrenfest theorem in this case, a fact that is already known for anti-hermitian QQM [1]. A real V implies that $\langle \mathbf{r} \rangle$ is dynamically classical and additionally that \mathcal{H} is hermitian; this constitutes further evidence that anti-hermitian operators may not be essential to QQM. (9) recovers the usual form of Ehrenfest theorem within the limit $\mathbf{Q} = \mathbf{0}$, where the usual linear momentum \mathbf{p} replaces $\mathbf{\Pi}$.

Let us then consider whether the expectation value of the linear momentum operator also behaves like the position expectation value. Along the x direction, we get

$$\frac{d\langle p_x \rangle}{dt} = - \left\langle \frac{\partial V}{\partial x} \right\rangle - V \frac{\partial \Psi}{\partial x} \Psi^* - iV\Psi \frac{\partial \Psi^*}{\partial x} i - \Psi \frac{\partial \Psi^*}{\partial x} V^* - i \frac{\partial \Psi}{\partial x} \Psi^* V^* i. \quad (11)$$

As in the case of $\langle x \rangle$, the expectation value generally does not behave classically, as the four terms in the right hand side of (11) demonstrate. We can get a better insight writing (10) as

$$\frac{d\langle p_x \rangle}{dt} = - \left\langle \frac{\partial V}{\partial x} \right\rangle - (V_0 - V_0^*) (Z - Z^*) - 2(V_1 W^* + W V_1^*), \quad (12)$$

where Z and W are obtained from the symplectic decomposition

$$\frac{\partial \Psi}{\partial x} \Psi^* = Z + Wj. \quad (13)$$

From (12) we clearly see that the expectation value of the momentum operator does behave according to classical dynamics for hermitian Hamiltonians, where V_0 is real and V_1 is zero. This means that QQM does satisfy the Ehrenfest theorem in the case of hermitian Hamiltonians, and the breakdown of the theorem for non-anti-hermitian operators is in agreement with anti-hermitian CQM. This enables us to infer that the origin of the breakdown of the classicality of $\langle x \rangle$ and $\langle p_x \rangle$ have the same origin, namely the non-hermiticity of the pure imaginary terms of the potential. Before considering the right complex wave equation case, let us consider several interesting properties of hermitian Hamiltonians in QQM. We notice that the time derivative of $\mathbf{\Pi}$ is too complicated so that its study and interpretation remain an open question.

A. Hermitian Hamiltonian operators

If \mathcal{H} is hermitian, it may be interchanged with $i\hbar\partial_t$, regardless of the wave function. Using this supposition, we use (1) and (8) to get the identity

$$\langle \mathcal{H}\mathcal{O} \rangle = \hbar \left\langle i \frac{\partial \mathcal{O}}{\partial t} \right\rangle - \langle i\mathcal{O}i\mathcal{H} \rangle. \quad (14)$$

Similar relations are obtained by replacing \mathcal{O} with $i\mathcal{O}i$, $\mathcal{O}i$ and $i\mathcal{O}$. From them, we eventually obtain

$$\begin{aligned}\langle [\mathcal{H}, \mathcal{O} - i\mathcal{O}i] \rangle &= \hbar \left\langle \frac{\partial}{\partial t} (\mathcal{O}i + i\mathcal{O}) \right\rangle, & \langle \{ \mathcal{H}, \mathcal{O} + i\mathcal{O}i \} \rangle &= -\hbar \left\langle \frac{\partial}{\partial t} (\mathcal{O}i - i\mathcal{O}) \right\rangle, \\ \langle [\mathcal{H}, \mathcal{O}i + i\mathcal{O}] \rangle &= -\hbar \left\langle \frac{\partial}{\partial t} (\mathcal{O} - i\mathcal{O}i) \right\rangle, & \langle \{ \mathcal{H}, \mathcal{O}i - i\mathcal{O} \} \rangle &= \hbar \left\langle \frac{\partial}{\partial t} (\mathcal{O} + i\mathcal{O}i) \right\rangle,\end{aligned}\quad (15)$$

where the square brackets denote commutation relations and the curly brackets denote anti-commutation relations. The set of relations (15) assures that the quaternionic solutions of (1) are stationary states. In other words, we have the Schrödinger picture, where wave functions are time-dependent and the operators are time-independent. At this point, it is natural to discuss the time evolution for the expectation values. Assuming (1) and (8), we get the identities

$$\frac{d}{dt} \langle \mathcal{O} - i\mathcal{O}i \rangle = \left\langle \frac{\partial}{\partial t} (\mathcal{O} - i\mathcal{O}i) \right\rangle + \frac{1}{\hbar} \langle [\mathcal{H}, \mathcal{O}i + i\mathcal{O}] \rangle + \frac{\partial}{\partial t} \langle \mathcal{O} - i\mathcal{O}i \rangle, \quad (16)$$

$$\frac{d}{dt} \langle \mathcal{O}i + i\mathcal{O} \rangle = \left\langle \frac{\partial}{\partial t} (\mathcal{O}i + i\mathcal{O}) \right\rangle - \frac{1}{\hbar} \langle [\mathcal{H}, \mathcal{O} - i\mathcal{O}i] \rangle + \frac{\partial}{\partial t} \langle \mathcal{O}i + i\mathcal{O} \rangle, \quad (17)$$

$$\frac{d}{dt} \langle \mathcal{O} + i\mathcal{O}i \rangle = \left\langle \frac{\partial}{\partial t} (\mathcal{O} + i\mathcal{O}i) \right\rangle - \frac{1}{\hbar} \langle \{ \mathcal{H}, \mathcal{O}i - i\mathcal{O} \} \rangle + \frac{\partial}{\partial t} \langle \mathcal{O} + i\mathcal{O}i \rangle, \quad (18)$$

$$\frac{d}{dt} \langle \mathcal{O}i - i\mathcal{O} \rangle = \left\langle \frac{\partial}{\partial t} (\mathcal{O}i - i\mathcal{O}) \right\rangle + \frac{1}{\hbar} \langle \{ \mathcal{H}, \mathcal{O} + i\mathcal{O}i \} \rangle + \frac{\partial}{\partial t} \langle \mathcal{O}i - i\mathcal{O} \rangle. \quad (19)$$

If \mathcal{O} and Ψ are complex, (16) and (17) recover the usual CQM relation, while (18) and (19) become trivial and the last term of the right hand side of each (16-19) disappears. This fact enables us to interpret that, in CQM, if (15) is valid then we will have stationary states.

Conversely, using (15) in (16-19) we calculate that the total time-derivatives are not identical to zero. Thus, the expectation values are not necessarily independent of time, nor are the wave functions stationary states. In order to obtain a quaternionic Schrödinger picture for LCWE we need the additional set of constraints, namely

$$\frac{\partial}{\partial t} \langle \mathcal{O} - i\mathcal{O}i \rangle = \frac{\partial}{\partial t} \langle \mathcal{O}i + i\mathcal{O} \rangle = \frac{\partial}{\partial t} \langle \mathcal{O} + i\mathcal{O}i \rangle = \frac{\partial}{\partial t} \langle \mathcal{O}i - i\mathcal{O} \rangle = 0. \quad (20)$$

Now, if (15) and (20) are valid, then we have stationary states and the quantum quaternionic states may be considered to be framed in the Schrödinger picture. A Heisenberg picture and the Virial theorem are also valid for hermitian Hamiltonian operators in the same fashion as in CQM, and thus QQM and CQM are perfectly compatible for hermitian Hamiltonians.

III. THE RIGHT COMPLEX WAVE EQUATION

In this section, we explore solutions of the quaternionic Schrödinger equation

$$\hbar \partial_t \Psi i = \mathcal{H} \Psi, \quad (21)$$

that we call the right complex wave function (RCWF). The terms of the continuity equation (5) obtained using (21) are

$$\rho = \Psi \Psi^*, \quad g = \frac{1}{\hbar} (i \Psi^* V^* \Psi - \Psi^* V \Psi i), \quad j = \frac{1}{2m} [\Psi^* \Pi \Psi + (\Psi^* \Pi \Psi)^*] \quad \text{and} \quad \Pi \Psi = -\hbar (\nabla - Q) \Psi i. \quad (22)$$

The source term of (22) presents an interesting feature, because quaternionic solutions may, in principle, be obtained considering $g = 0$ as a constraint. To our knowledge, these solutions have never been studied, and this would seem to be an interesting direction for future research. Taking inspiration from the probability current (22), we propose the expectation value for the RCWF

$$\langle \mathcal{O} \rangle = \frac{1}{2} \int dx^3 [\Psi^* \mathcal{O} \Psi + (\Psi^* \mathcal{O} \Psi)^*]. \quad (23)$$

We can study the Ehrenfest theorem using (23), and consequently

$$\frac{d\langle \mathbf{r} \rangle}{dt} = \frac{\langle \Pi \rangle}{m} - \frac{2}{\hbar} \langle (V \mathbf{r} | i) \rangle, \quad (24)$$

where we define the notation

$$(\mathcal{O}|i)\Psi = \mathcal{O}\Psi i \quad (25)$$

As in the left complex wave function, the second term on the right hand side of (24) are zero for real V , and the dynamics of $\langle x \rangle$ is classical for hermitian Hamiltonians as well. Now we will study the time evolution for the momentum operator along the x direction, so that

$$\frac{d\langle p_x \rangle}{dt} = -\left\langle \frac{\partial_x V}{\partial x} \right\rangle + \langle (V^* - V)\partial_x \rangle. \quad (26)$$

Again, we have a perfect agreement with the LCWF for quaternionic potentials and an agreement with CQM for real potentials.

A. Hermitian Hamiltonian operators

A hermitian Hamiltonian enables us to obtain

$$\left\langle [(\mathcal{H}|i), \mathcal{O}] \right\rangle = -\hbar \left\langle \frac{\partial}{\partial t} \mathcal{O} \right\rangle, \quad (27)$$

and we observe that there are important differences compared to the LCWF: there is only one equation and there are no anti-commutation relations. We expect that the physical content of the left complex case is different from the right complex case, but the actual differences will only be ascertained after explicit solutions have been found. Finally, we get

$$\frac{d}{dt} \langle \mathcal{O} \rangle = \left\langle \frac{\partial}{\partial t} \mathcal{O} \right\rangle + \frac{1}{\hbar} \left\langle [(\mathcal{H}|i), \mathcal{O}] \right\rangle + \frac{\partial \langle \mathcal{O} \rangle}{\partial t}. \quad (28)$$

As in the LCWE, stationary states are obtained if a set of constraints include (27) and

$$\frac{\partial \langle \mathcal{O} \rangle}{\partial t} = 0. \quad (29)$$

Hence we have a consistent QQM for the RCWE, which contains a wave equation, a continuity equation and a classical limit. In future research, we will develop explicit solutions to illustrate and build models where some physical phenomena can be researched. However, the important point of the formal consistent has been established throughout this study.

IV. CONCLUSION

In this article, we have proposed an alternative formulation for quaternionic quantum mechanics that has enabled us to explain the breakdown of the Ehrenfest theorem observed in the anti-hermitian formulation of QQM. This formulation of QQM encompasses quaternionic Hamiltonians, and neither hermiticity nor anti-hermiticity are supposed. In spite of this, we were able to define a theory with real-value expectation values.

The existence of either sources or sinks of density of probability has been ascertained to be responsible for the breakdown of the Ehrenfest theorem, and these sources of probability density are generated by the imaginary terms of the scalar potential of the Hamiltonian operator.

The results indicate that meaningful quantum quaternionic effects can be researched in physical situations that are found in non-hermitian CQM, like resonances and scattering phenomena [4, 5]. Another important possible source of interesting physics problems involves geometric phases, and an initial theoretical study has already been conducted [2]. Measurable effects have never been researched for non-hermitian quaternionic physical situations, and we expect that the framework we propose may be useful for renewing the interest in QQM within the field of experimental physics. On the other hand, we hope that theoretical interest in quaternionic quantum solutions may also be renewed, particularly the search for explicit solutions.

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